On a general solution of the one-dimensional stationary Schrödinger equation

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Abstract

The general solution of the one-dimensional stationary Schrödinger equation in the form of a formal power series is considered. Its efficiency for numerical analysis of initial value and boundary value problems is discussed.

Consider the equation

$$(pu')' + qu = \omega^2 u \tag{1}$$

where we suppose that p, q and u are complex-valued functions of an independent real variable $x \in [0, a]$, ω is an arbitrary complex number. p and q are supposed to be such that there exists a solution g_0 of the equation $(pg_0')' + qg_0 = 0$ on $(0, a)$ such that $g_0 \in C^2(0, a)$ together with $1/g_0$ are bounded on $[0, a]$ and $p \in C^1(0, a)$ is a bounded nonvanishing function on $[0, a]$. Denote $g = \sqrt{p}g_0$. In [3] with the aid of pseudoanalytic function theory [2] the following result was obtained.

Theorem 1 *The general solution of (1) has the form*

$$u = c_1 u_1 + c_2 u_2 \tag{2}$$

where c_1 and c_2 are arbitrary complex constants, u_1 and u_2 are defined as follows

$$u_1 = g_0 \sum_{\text{even } n=0}^{\infty} \frac{\omega^n}{n!} \widetilde{X}^{(n)} \quad \text{and} \quad u_2 = g_0 \sum_{\text{odd } n=1}^{\infty} \frac{\omega^n}{n!} X^{(n)} \tag{3}$$

where $\widetilde{X}^{(n)}$ and $X^{(n)}$ are introduced by the following recurrent equalities

$$\widetilde{X}^{(0)} \equiv 1, \quad X^{(0)} \equiv 1, \tag{4}$$

and for $n \in \mathbb{N}$,

$$\widetilde{X}^{(n)}(x) = \begin{cases} n \int\limits_0^x \widetilde{X}^{(n-1)}(\xi) g_0^2(\xi) d\xi & \text{for an odd } n \\ n \int\limits_0^x \widetilde{X}^{(n-1)}(\xi) g^{-2}(\xi) d\xi & \text{for an even } n \end{cases} \tag{5}$$

$$X^{(n)}(x) = \begin{cases} n \int\limits_0^x X^{(n-1)}(\xi) g^{-2}(\xi) d\xi & \text{for an odd } n \\ n \int\limits_0^x X^{(n-1)}(\xi) g_0^2(\xi) d\xi & \text{for an even } n \end{cases} \tag{6}$$

Another representation of the general solution of (1) as a formal power series has been known since quite long ago (see [4, Theorem 1]) and used for studying qualitative properties of solutions. The parameter ω participated in that representation in a very complicated manner which made that form of a general solution too difficult to be used for quantitative analysis of spectral and boundary value problems. To the contrast, the solution (2), (3) is a power series with respect to ω which makes it really attractive for numerical solution of spectral, initial value and boundary value problems.

The required for (3) particular solution g_0 can be constructed in a similar way. By analogy with theorem 1 the following result can be obtained.

Theorem 2 *Suppose that $q \in C[0, a]$. The general solution of the equation*

$$-\frac{d^2u(x)}{dx^2} + q(x)u(x) = 0 \tag{7}$$

on $(0, a)$ *has the form*

$$u = c_1 u_1 + c_2 u_2 \tag{8}$$

where c_1 *and* c_2 *are arbitrary constants;* u_1*,* u_2 *are defined as follows*

$$u_1 = \sum_{\textit{even } n=0}^{\infty} \frac{\widetilde{X}^{(n)}}{n!} \qquad \textit{and} \qquad u_2 = \sum_{\textit{odd } n=1}^{\infty} \frac{X^{(n)}}{n!}. \tag{9}$$

and $\widetilde{X}^{(n)}$*,* $X^{(n)}$ *are introduced by the following recurrent equalities*

$$\widetilde{X}^{(0)} \equiv 1, \quad X^{(0)} \equiv 1, \tag{10}$$

and for $n \in \mathbb{N}$*,*

$$\widetilde{X}^{(n)}(x) = \begin{cases} n \int\limits_0^x \widetilde{X}^{(n-1)}(\xi) d\xi & \text{for an even } n \\ n \int\limits_0^x \widetilde{X}^{(n-1)}(\xi) q(\xi) d\xi & \text{for an odd } n \end{cases} \tag{11}$$

$$X^{(n)}(x) = \begin{cases} n \int\limits_0^x X^{(n-1)}(\xi) q(\xi) d\xi & \text{for an even } n \\ n \int\limits_0^x X^{(n-1)}(\xi) d\xi & \text{for an odd } n \end{cases} \tag{12}$$

Proof. First of all let us verify that both series are uniformly convergent on the considered interval. For this purpose we notice that for an even n,

$$\left| \widetilde{X}^{(n)}(x) \right| \le \left(\max_{x \in [0,x]} |q(x)| \right)^{n/2} x^n \le \left(\max_{x \in [0,a]} |q(x)| \right)^{n/2} a^n.$$

Thus, the members of the series in u_1 can be estimated by constants: $\frac{\left|\widetilde{X}^{(n)}(x)\right|}{n!} \le \frac{\left(\max_{x\in[0,a]}|q(x)|\right)^{n/2} a^n}{n!}$ for any $x \in [0, a]$ and the series $\frac{c^n}{n!}$ converges where $c = \left(\max_{x\in[0,a]} |q(x)|\right)^{1/2} a$. Then by the Weierstrass theorem the series in u_1 is uniformly convergent. The uniform convergence of the series in u_2 (as well as of the series of derivatives) can be shown by analogy.

Now we can apply the operator $\frac{d^2}{dx^2}$ to each of the series. Note that for an even $n > 0$,

$$\frac{d^2}{dx^2}\widetilde{X}^{(n)} = n\frac{d}{dx}\widetilde{X}^{(n-1)} = (n-1)nq\widetilde{X}^{(n-2)}.$$

Thus,

$$\frac{d^2}{dx^2}u_1 = q\sum_{\text{even } n=2}^{\infty}\frac{\widetilde{X}^{(n-2)}}{(n-2)!} = q\sum_{\text{even } n=0}^{\infty}\frac{\widetilde{X}^{(n)}}{n!} = qu_1.$$

For an odd $n > 1$ (obviously, $\frac{d^2X^{(1)}}{dx^2} = 0$) we have

$$\frac{d^2}{dx^2}X^{(n)} = n\frac{d}{dx}X^{(n-1)} = (n-1)nqX^{(n-2)}.$$

And consequently

$$\frac{d^2}{dx^2}u_2 = q\sum_{\text{odd } n=3}^{\infty}\frac{X^{(n-2)}}{(n-2)!} = q\sum_{\text{odd } n=1}^{\infty}\frac{X^{(n)}}{n!} = qu_2.$$

Thus, u_1 and u_2 are solutions of (7). Last step is to verify that their Wronskian is different from zero at least at one point. It is easy to see that the Wronskian has the form

$$\left(\sum_{\text{even } n=0}^{\infty}\frac{\widetilde{X}^{(n)}}{n!}\right)\left(\sum_{\text{even } m=0}^{\infty}\frac{X^{(m)}}{m!}\right) - \left(\sum_{\text{odd } n=1}^{\infty}\frac{\widetilde{X}^{(n)}}{n!}\right)\left(\sum_{\text{odd } m=1}^{\infty}\frac{X^{(m)}}{m!}\right).$$

At the point zero all $X^{(m)}$ and $\widetilde{X}^{(n)}$ vanish except for $X^{(0)}$ and $\widetilde{X}^{(0)}$. Thus the Wronskian is equal to 1 at $x = 0$ and hence the functions u_1, u_2 are linearly independent that finishes the proof. $\blacksquare$

This theorem in different, quite more difficult notations was known already at the beginning of the last century (see [8]) and was also used for qualitative analysis of solutions of (7). Nevertheless here we want to emphasize the extreme usefulness of theorem 2 as well as of theorem 1 for numerical solution of initial value and boundary value problems for second-order linear differential equations, which escaped attention of researchers working in numerical solution of ordinary differential equations. First of all, let us notice that in (8) $c_1 = u(0)$ and $c_2 = u'(0)$. That is the representation of a general solution (8), (9) is very convenient for solving initial value problems.

We remind that solution of boundary value problems for (7) reduces to solving a couple of initial value problems (see, e.g., [6]), so this property of the representation (8), (9) is well suited for solving boundary value problems as well.

Moreover, note that very often, e.g., in electromagnetic theory (see, [7]) it is necessary to solve the equation

$$-\frac{d^2u(x)}{dx^2}+\omega^2 q(x)u(x)=0 \tag{13}$$

for different values of the complex constant ω^2. According to theorem 2 its general solution can be represented as follows

$$u=c_1\sum_{\text{even } n=0}^{\infty}\frac{\omega^n\widetilde{X}^{(n)}}{n!}+c_2\sum_{\text{odd } n=1}^{\infty}\frac{\omega^{n-1}X^{(n)}}{n!}$$

with $X^{(n)}$ and $\widetilde{X}^{(n)}$ defined by (10)-(12). Thus, once $X^{(n)}$ and $\widetilde{X}^{(n)}$ up to a certain order N are calculated, an approximate solution of (13) is just a polynomial in ω with calculated coefficients $X^{(n)}$ and $\widetilde{X}^{(n)}$. This observation is also valid in the case of the solution (2), (3) of equation (1). This property is very useful for numerical solution of corresponding spectral problems which then reduces to finding zeros of polynomials with respect to ω. In the present work we are more interested in studying the convergence and accuracy of the numerical method based on representations of the form (8), (9) in comparison with known standard algorithms.

An important feature of the representation (8), (9) is that it is well suited for symbolic calculations in principle in a general case. The coefficient q can be interpolated arbitrarily accurately by means of a polynomial or splines and then all integrations in (11) and (12) can be done symbolically in a package like Mathematica or Maple. In the present work we made use of Matlab 7 and compared our results with standard Matlab ODE solvers [1], [5], especially with ode45 which in the considered examples gave always better results than other similar programs.

Consider the following initial value problem for (7): $q\equiv -c^2$, $u(0)=1$, $u'(0)=-1$ on the interval $(0,1)$. For $c=1$ the absolute error of the result calculated by ode45 (with an optimal tolerance chosen) was of order 10^{-9} and the relative error was of order 10^{-6} meanwhile the absolute error of the result calculated with the aid of theorem 2 with N (the number of formal

powers in the truncated series (9)) from 55 to 58 was of order 10^{-16} and the relative error was of order 10^{-14}. Taking $c = 10$ under the same conditions the absolute and the relative errors of ode45 were of order 10^{-6} and 10^{-5} respectively meanwhile our algorithm based on theorem 2 gave values of order 10^{-12} in both cases.

For the initial value problem: $q \equiv c^2$, $u(0) = 1$, $u'(0) = -1$ on the interval $(0, 1)$ in the case $c = 1$ the absolute and the relative errors of ode45 were of order 10^{-8} meanwhile in our method this value was of order 10^{-15} already for $N = 50$. For $c = 10$ the absolute and the relative errors of ode45 were of order 10^{-3} and 10^{-7} respectively and in the case of our method these values were of order 10^{-11} and 10^{-14} for $N = 50$.

Consider another example. Let $q(x) = c^2x^2 + c$. In this case the general solution of (7) has the form

$$u(x) = e^{cx^2/2}\left(c_1 + c_2\int_0^x e^{-ct^2}dt\right).$$

Take the same initial conditions as before, $u(0) = 1$, $u'(0) = -1$. Then meanwhile for $c = 1$ the absolute and the relative error of ode45 was of order 10^{-8} and for $c = 30$ the absolute error was 0.28 and the relative error was of order 10^{-6}, our algorithm ($N = 58$) gave the absolute and relative errors of order 10^{-15} for $c = 1$ and the absolute and relative errors of order 10^{-9} and 10^{-15} respectively for $c = 30$. All calculations were performed on a usual PC with the aid of Matlab 7.

The results of our numerical experiments show that in fact theorem 1 and theorem 2 offer a new powerful method for numerical solution of initial value and boundary value problems for linear ordinary differential second-order equations. Numerical calculation of integrals involved in (5), (6) and in (11), (12) does not represent any considerable difficulty and can be done with a remarkable accuracy.

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